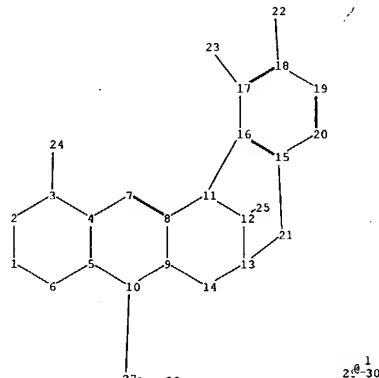
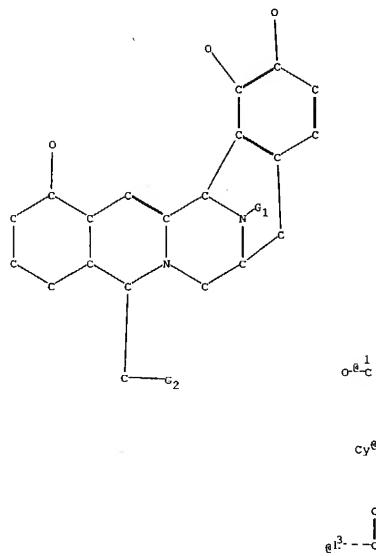


CAS. Part 2 /D  
(Claim, 33, etc.)



FOR  
CLAIM 33, etc.

chain nodes :  
22 23 24 25 27 28 29 31 34

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21

ring/chain nodes :

30 32 33

chain bonds :

3-24 10-27 12-25 17-23 18-22 27-28 29-30 32-33 33-34

ring bonds :

1-2 1-6 2-3 3-4 4-5 4-7 5-6 5-10 7-8 8-9 8-11 9-10 9-14 11-12 11-16 12-13  
13-14 13-21 15-16 15-20 15-21 16-17 17-18 18-19 19-20

exact/norm bonds :

1-2 1-6 2-3 3-4 3-24 4-5 4-7 5-6 5-10 7-8 8-9 8-11 9-10 9-14 11-12 11-16  
12-13 12-25 13-14 13-21 15-21 17-23 18-22 27-28 29-30 32-33 33-34

exact bonds :

10-27

normalized bonds :

15-16 15-20 16-17 17-18 18-19 19-20

isolated ring systems :

containing 1 :

1:H,CH3

2:H,OH,[\*1],[\*2],[\*3]

match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom  
12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom 21:Atom  
22:CLASS 23:CLASS 24:CLASS 25:CLASS 27:CLASS 28:CLASS 29:CLASS 30:CLASS 31:Atom  
32:CLASS 33:CLASS 34:CLASS

generic attributes :

31:

Saturation : Unsaturated

10/728580

=> file caplus  
COST IN U.S. DOLLARS  
FULL ESTIMATED COST

	SINCE FILE ENTRY	TOTAL SESSION
	155.84	156.05

FILE 'CAPLUS' ENTERED AT 19:03:05 ON 20 NOV 2004  
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.  
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.  
COPYRIGHT (C) 2004 AMERICAN CHEMICAL SOCIETY (ACS)

Copyright of the articles to which records in this database refer is held by the publishers listed in the PUBLISHER (PB) field (available for records published or updated in Chemical Abstracts after December 26, 1996), unless otherwise indicated in the original publications. The CA Lexicon is the copyrighted intellectual property of the American Chemical Society and is provided to assist you in searching databases on STN. Any dissemination, distribution, copying, or storing of this information, without the prior written consent of CAS, is strictly prohibited.

FILE COVERS 1907 - 20 Nov 2004 VOL 141 ISS 22  
FILE LAST UPDATED: 18 Nov 2004 (20041118/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> d his

(FILE 'HOME' ENTERED AT 19:01:56 ON 20 NOV 2004)

FILE 'REGISTRY' ENTERED AT 19:02:05 ON 20 NOV 2004

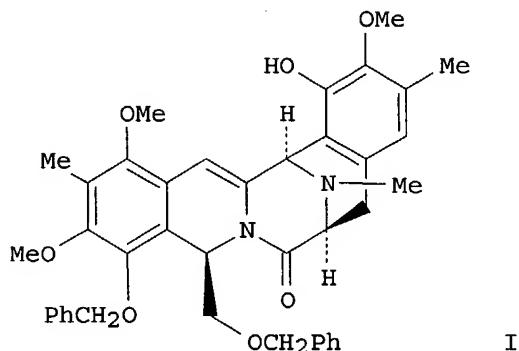
L1                   STRUCTURE UPLOADED  
L2                   0 S L1  
L3                   4 S L1 SSS FULL

FILE 'CAPLUS' ENTERED AT 19:03:05 ON 20 NOV 2004

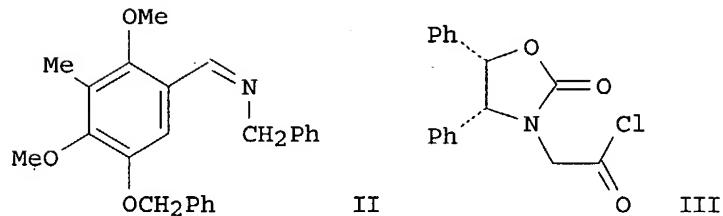
=> s 13  
L4                   2 L3

=> d 14 1-2 bib abs hitstr

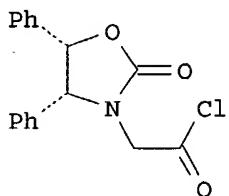
L4 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2004 ACS on STN  
 AN 2003:382225 CAPLUS  
 DN 139:101312  
 TI Synthetic Studies on Ecteinascidin-743: Constructing a Versatile  
 Pentacyclic Intermediate for the Synthesis of Ecteinascidins and  
 Saframycins  
 AU Jin, Wei; Metobo, Sammy; Williams, Robert M.  
 CS Department of Chemistry, Colorado State University, Fort Collins, CO,  
 80523, USA  
 SO Organic Letters (2003), 5(12), 2095-2098  
 CODEN: ORLEF7; ISSN: 1523-7060  
 PB American Chemical Society  
 DT Journal  
 LA English  
 OS CASREACT 139:101312  
 GI



I



II



III

AB The asym. synthesis of a highly functionalized pentacyclic  
 tetrahydroisoquinoline, I, relevant to the ecteinascidin, saframycin,  
 safracin, and renieramycin family of antitumor alkaloids is described. I  
 was prepared via Staudinger reaction of imine II with the ketene of acid  
 chloride III and a Pictet-Spengler cyclization.

IT 557785-63-4P

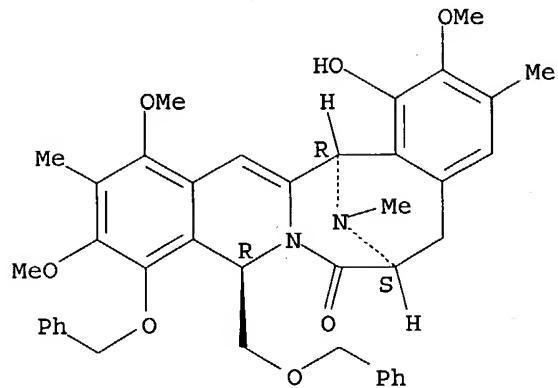
RL: SPN (Synthetic preparation); PREP (Preparation)  
 (asym. synthesis of pentacyclic isoquinoline as intermediate for  
 ecteinascidins and saframycins via Staudinger and Pictet-Spengler  
 reactions)

RN 557785-63-4 CAPLUS

CN 6,15-Imino-7H-isoquinolo[3,2-b][3]benzazocin-7-one, 5,6,9,15-tetrahydro-1-  
 hydroxy-2,11,13-trimethoxy-3,12,16-trimethyl-10-(phenylmethoxy)-9-  
 [(phenylmethoxy)methyl]-, (6S,9R,15R)- (9CI) (CA INDEX NAME)

10/728580

Absolute stereochemistry: Rotation (-).

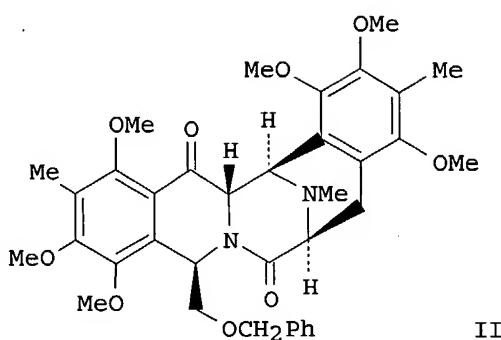
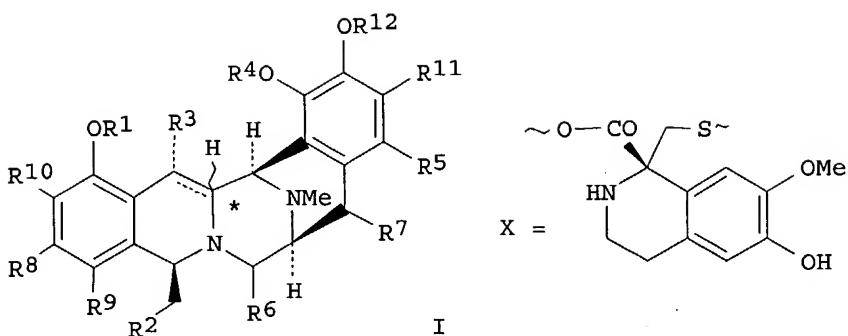


RE.CNT 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

10/728580

L4 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2004 ACS on STN  
AN 2001:545697 CAPLUS  
DN 135:137633  
TI Preparation of saframycin-ecteinascidin analogs and their therapeutic applications  
IN Danishefsky, Samuel J.; Zhou, Bishan  
PA The Trustees of Columbia University in the City of New York, USA  
SO PCT Int. Appl., 115 pp.  
CODEN: PIXXD2  
DT Patent  
LA English  
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2001053299	A1	20010726	WO 2001-US1877	20010119
	WO 2001053299	C2	20021024		
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
	CA 2397597	AA	20010726	CA 2001-2397597	20010119
	US 2002025962	A1	20020228	US 2001-765515	20010119
	US 6686470	B2	20040203		
	EP 1254140	A1	20021106	EP 2001-903151	20010119
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
	JP 2003520801	T2	20030708	JP 2001-553773	20010119
	US 2004127709	A1	20040701	US 2003-728580	20031205
PRAI	US 2000-177071P	P	20000119		
	US 2001-765515	A3	20010119		
	WO 2001-US1877	W	20010119		
OS	MARPAT	135:137633			
GI					



AB Compds. of the saframycin-ecteinascidin series such as I [R1,R4 = H, alkyl, acyl; R3 = =O, OH, ether, sulfide, acyl group such as OC(O)Me, OC(O)Bn and OC(O)Et; R5 = H, halogen, OH, ether, acyl, amide; R6 = =O, OH, OMe, CN, acyloxy; R7 = =O, OH, halogen, ether, acyl; R8 and R9 independently = H, Me, OMe, OEt, CF<sub>3</sub>, Br, F; R8R9 = OCH<sub>2</sub>O, five or six membered ring; R10,R11 = Me, OMe, OEt, SMe, SEt; R12 = H, alkyl, acyl; chiral center marked \* has the R or the S configuration], were prepared for use as antitumor and antimicrobial agents. Thus, saframycin analog II was prepared via a multistep synthetic sequence starting from 2,4-Dimethoxy-3-methylbenzaldehyde, bromoacetal, 2-hydroxy-4-methoxy-3-methylbenzaldehyde and [(2E)-4-bromo-2-butenyl]oxy] (1,1-dimethylethyl)dimethylsilane. Ecteinascidin 743 I (R1 = Ac, R2R3 = X, R4 = R5 = R7 = H, R6 =  $\alpha$ -OH, R8R9 = OCH<sub>2</sub>O, R10-R12 = Me) was tested for cytotoxicity and antimicrobial activity.

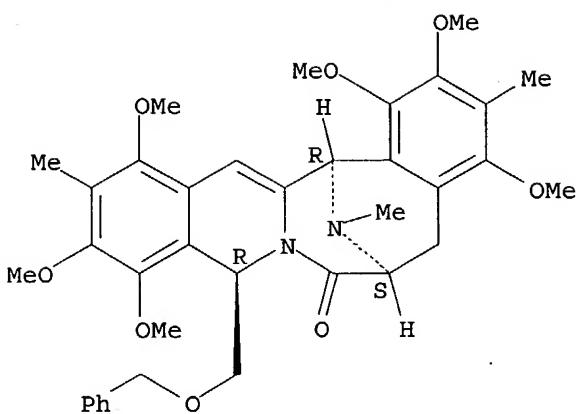
IT 351377-82-7P 351378-34-2P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (preparation of saframycin-ecteinascidin analogs and their therapeutic applications)

RN 351377-82-7 CAPLUS

CN 6,15-Imino-7H-isoquinol[3,2-b][3]benzazocin-7-one, 5,6,9,15-tetrahydro-1,2,4,10,11,13-hexamethoxy-3,12,16-trimethyl-9-[(phenylmethoxy)methyl]-, (6S,9R,15R)- (9CI) (CA INDEX NAME)

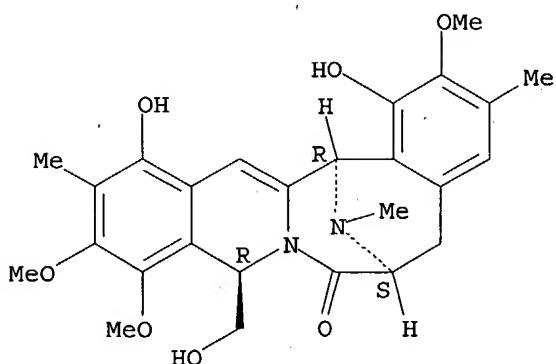
Absolute stereochemistry.



RN 351378-34-2 CAPLUS

CN 6,15-Imino-7H-isoquinolo[3,2-b][3]benzazocin-7-one, 5,6,9,15-tetrahydro-1,13-dihydroxy-9-(hydroxymethyl)-2,10,11-trimethoxy-3,12,16-trimethyl-, (6S,9R,15R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 351377-80-5P

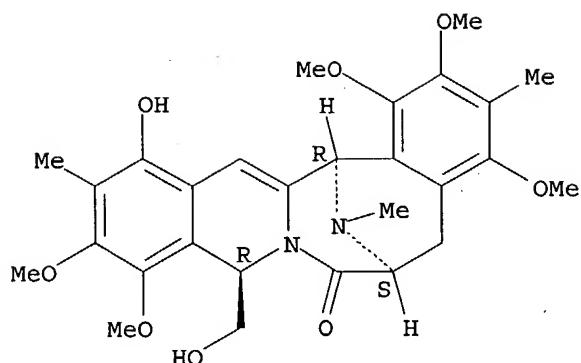
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation of saframycin-ecteinascidin analogs and their therapeutic applications)

RN 351377-80-5 CAPLUS

CN 6,15-Imino-7H-isoquinolo[3,2-b][3]benzazocin-7-one, 5,6,9,15-tetrahydro-13-hydroxy-9-(hydroxymethyl)-1,2,4,10,11-pentamethoxy-3,12,16-trimethyl-, (6S,9R,15R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

10/728580



RE.CNT 2

THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

10/728580

=> file caold		
COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	10.40	166.45
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
CA SUBSCRIBER PRICE	-1.40	-1.40

FILE 'CAOLD' ENTERED AT 19:04:01 ON 20 NOV 2004  
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.  
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.  
COPYRIGHT (C) 2004 AMERICAN CHEMICAL SOCIETY (ACS)

FILE COVERS 1907-1966  
FILE LAST UPDATED: 01 May 1997 (19970501/UP)

This file contains CAS Registry Numbers for easy and accurate substance identification. Title keywords, authors, patent assignees, and patent information, e.g., patent numbers, are now searchable from 1907-1966. TIFF images of CA abstracts printed between 1907-1966 are available in the PAGE display formats.

This file supports REG1stRY for direct browsing and searching of all substance data from the REGISTRY file. Enter HELP FIRST for more information.

=> s 13  
L5 0 L3

=> log h		
COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	0.42	166.87
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
CA SUBSCRIBER PRICE	0.00	-1.40

SESSION WILL BE HELD FOR 60 MINUTES  
STN INTERNATIONAL SESSION SUSPENDED AT 19:04:09 ON 20 NOV 2004